Nondestructive assessment of quality of Nanfeng mandarin fruit by a portable near infrared spectroscopy

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Abstract: A portable near infrared spectroscopy system was developed for assessing the quality of Nanfeng mandarin fruit. One hundred and fifty-three Nanfeng mandarin samples were used to measure the performance of the system. Several pretreatment methods were adopted to process the spectra. Then Support Vector Machine (SVM), Back Propagation Neural Network (BPNN) and Partial Least Square (PLS) were used to build models for soluble solids content (SSC), titratable acidity (TA), vitamin C and surface color. The best results were obtained by SVM. The correlation coefficient (R) and root mean square error of prediction (RMSEP) were (0.93, 0.65°Brix), (0.66, 0.09%), (0.81, 2.7mg/100g) and (0.57, 0.81) for SSC, TA, vitamin C and color, respectively. The results demonstrated that the portable near infrared spectroscopy was feasible for determining the Nanfeng mandarin quality nondestructively.

Keywords: Portable near infrared spectroscopy, SVM, Nanfeng mandarin fruit, SSC, TA, Vitamin C, surface color

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1 Introduction

Fruit quality is a vital factor that affects its market value, its transportation and storage requirements. Basically, fruit quality indices consist of internal and external quality, such as soluble solids content (SSC), titratable acidity (TA), firmness, vitamin C, surface color, shape and appearance. The fruit is graded by the external quality, including surface color, size and surface defects[1-3]. However, determination of the internal quality is not as straightforward as the external quality measurement. The composition and the texture condition of fruit are usually measured by destructive or invasive approaches which involve a considerable amount of manual work.

Near infrared spectroscopy (NIR) technique, combining with chemometrics algorithms, is a powerful tool because of its fast measurement and simple operation in sampling. Thus, NIR has been applied to assess nondestructively the quality indices of mandarin or citrus fruit, such as SSC[4-9], SSC and TA[10], SSC, TA and firmness[11], defect and ripeness[12]. Even if these instruments are highly precise, their application to field research, such as monitoring of chemical changes of developing fruits on trees, are limited by their large sizes and weights. Presently, several portable NIR instruments are commercially available for determining SSC value. Saranwong et al. (2003) reported that the accuracy of the Kubota NIR instrument “Fruit Selector” for SSC value determination of intact mango was 0.40°Brix in SEP[13]. The research by Temma et al (2002) also showed that the portable NIR instrument developed by their research centre had excellent potential in determining SSC value of intact apples[14]. Camps et al. (2009) [15] developed a portable NIR instrument for determining SSC, TA and firmness of apricots with a miniature optical component

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(S-2000). So it is necessary to investigate the performance of the portable NIR instrument[15].

The objectives of this study were to build a portable NIR system with the miniature optical components, and to investigate the performance for evaluating the Nanfeng mandarin fruit quality nondestructively, including SSC, TA, vitamin C and color. To obtain steady models, SVM, BPNN and PLS methods were tried.

2 Materials and methods

2.1 Nanfeng mandarin fruit

One hundred and fifty-three Nanfeng mandarin fruits were harvested from a local orchard in Jiangxi Province. They were placed in airtight polyethylene bags and stored in an ice filled refrigerator to keep at cold temperature (4±1)℃. All fruit samples were allowed to equilibrate to room temperature (20℃) for one day before NIRS measurement. SSC, TA and vitamin C were measured by traditional destructive tests. Each fruit unit was juiced and SSC was obtained using a Digital Refractometer PR-101α (Atago Co. Ltd., Tokyo, Japan). TA was assessed by potentiometric titration of a 2 mL sample of juice and expressed as percentage of citric aid. Vitamin C was titrated manually by 2,6-Dichloroindophenol titration method. Color was measured by CIELAB (MINOLTA CR-10, Konica Minolta, Inc., Osaka, Japan). And the data set was divided into calibration and prediction sets (110:43). Because of errors in invasive measurement, abnormal samples were eliminated. The data of calibration and prediction set are presented in Table 1.

Table 1 Number of samples, mean and range in calibration and prediction set for different quality indices

Quality indices	Calibration set			Prediction set		
	Number	Mean	Range	Number	Mean	Range
SSC/°Brix	107	13.90)	9.60-18.00	43	14.00	10.50-17.90
TA/%	104	0.45	0.22-0.94	42	0.45	0.23-0.92
vitamin C/mg・(100 g)$^{-1}$	98	15.5	4.1-27.0	41	14.6	6.1-26.5
color (△*E*)	102	78.60	76.00-81.00	37	78.50	76.60-80.50

$\Delta E = \sqrt{L^2 + a^2 + b^2}$, △*E* is defined by CIELAB 1976.

2.2 System setup and measurements

The system consisted of a tungsten halogen lamp (24V/50W), a miniature CCD spectrometer (USB4000), an optical fiber (SMA905), a USB data line and a computer. The CCD spectrometer was 3648 pixel photodiode array. The wavelength range of the spectrometer was 400−1040 nm with a 0.2 sampling interval. The angle was 30 degrees between the lamp axis and the vertical line[16,17]. The horizontal distance was about 150 mm between the center of lamp and fruit holder.

NIR spectra were collected and transformed by OOIBase32 software (Oceanoptics Inc., Dunedin, Florida USA). A spectrum was collected after the fruit were rotated every 120 degrees. The spectra were analyzed by ‘Unscrambler V8.0 software (CAMO, Trondheim, Norway) and Matlab 7.0 software (Mathworks, Natick, USA).

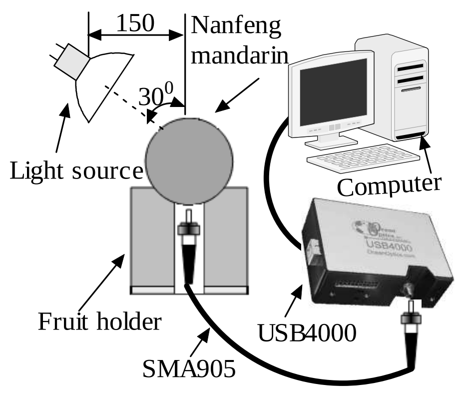

Figure 1 Schematic diagram of Nanfeng mandarin NIRS acquisition device

2.3 Model evaluation

The performance of the models was evaluated in terms of the root mean square error of calibration (RMSEC), the root mean square error of prediction (RMSEP) and the correlation coefficient (R), respectively. The RMSECV was calculated as follows:

$$RMSEC = \sqrt{\frac{1}{n_c - 1}\sum_{i=1}^{n_c}(\hat{y}_i - y_i)^2} \quad (1)$$

where $\hat{y}_i$ is the prediction value of the i th observation; y_i is the measured value of i th observation and n_c is the number of the observations in the calibration set.

For the prediction set, the RMSEP was calculated as follows:

$$RMSEP = \sqrt{\frac{\sum_{i=1}^{n_p}(y_i - \hat{y}_i)^2}{n_p}} \quad (2)$$

where $\hat{y}_i$ is the prediction value of the i th observation; y_i is the measured value of the i th observation and n_p is the number of the observations in the prediction set.

Correlation coefficients between the prediction and the measurement value were calculated as follows:

$$r = \sqrt{\frac{\sum_{i=1}^{n}(\hat{y}_i - y_i)^2}{\sum_{i=1}^{n}\left(\hat{y}_i - \bar{y}\right)^2}} \quad (3)$$

where $\hat{y}_i$, y_i are the prediction and measurement value of sample i in the calibration and prediction sets; $\bar{y}$ is the mean of the reference measurement results for all samples in calibration and prediction sets and n is the number of the observations in calibration and prediction set.

The ideal model should have the higher R value and the lower RMSEC, RMSEP and RSE values, and the RMSEC is almost close to the RMSEP.

3 Results and discussion

3.1 NIR spectra

Absorption or scatter of incident radiation is dependent upon physical and chemical characteristics of the mandarin fruits, such as density, size, water content, SSC, presence of seeds, color, etc. Several absorption peaks appeared in the spectra of Nanfeng mandarin fruits, the typical spectra are shown in Figure 2. The presence of a chlorophyll absorbance was observed as a slight inflexion point at around 680 nm. The presence of strong water absorbance bands were observed at around 710 nm and 960 nm, because of the third and second harmonics of the fundamental OH stretching vibration. An inflexion point was observed at 810 nm, because of the second harmonic of a combinational OH stretching and bending vibration.

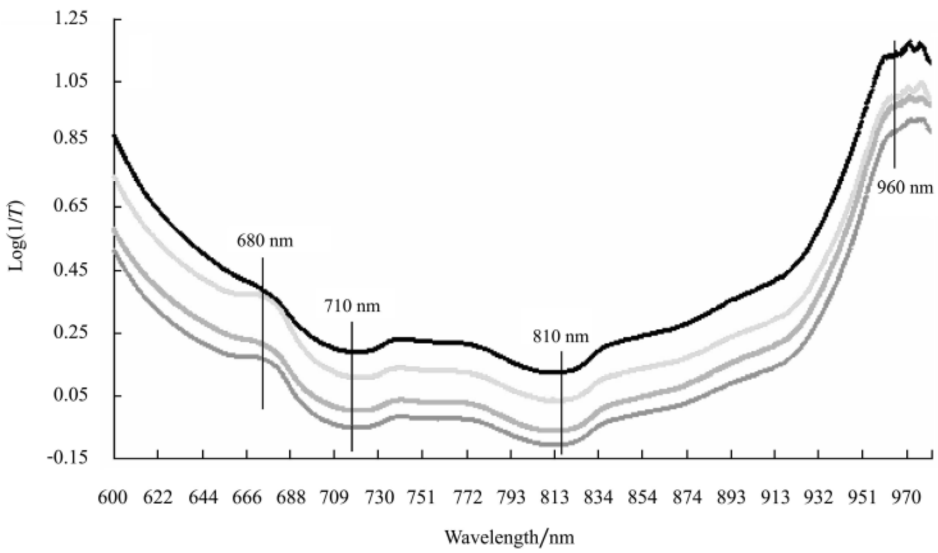

Figure 2 Typical spectra of Nanfeng mandarin fruits

3.2 Pretreatment methods

The NIR spectra often require mathematical pretreatment to remove interference of specular radiation, such as smooth, multiplicative scatter correction (MSC), first derivative and second derivative. The pretreatment methods were attempted to eliminate the interference by smooth, MSC, first derivative and second derivative, respectively. The results are shown in Table 2. The results without pretreatment methods were better. This was probably due to the advantages of the transmission mode over reflectance. In transmission mode, a direct measurement of the bulk flesh properties was undertaken, and there was not specularly reflected background radiation interfering with the results[18].

Table 2 Statistical results with different pre-process methods

Indices	Spectrum Pretreatment	LVs	Calibration set		Prediction set	
			R	*RMSEC*	*r*	*RMSEP*
SSC	None	14	0.94	0.53	0.92	0.65
	Savitzky-Golay	16	0.94	0.53	0.91	0.72
	1st Derivative	12	0.95	0.49	0.83	0.91
	2nd Derivative	14	0.95	0.50	0.85	0.87
	MSC	14	0.96	0.46	0.92	0.66
TA	None	5	0.65	0.10	0.64	0.09
	Savitzky-Golay	5	0.65	0.10	0.65	0.09
	1st Derivative	4	0.65	0.10	0.62	0.10
	2nd Derivative	4	0.63	0.10	0.61	0.10
	MSC	7	0.73	0.09	0.66	0.09
Vitamin C	None	8	0.80	3.3	0.80	2.8
	Savitzky-Golay	8	0.80	3.3	0.80	2.8
	1st Derivative	3	0.73	3.7	0.73	3.2
	2nd Derivative	4	0.75	3.6	0.69	3.3
	MSC	6	0.78	3.4	0.75	3.1
Surface color	None	4	0.57	0.84	0.53	0.82
	Savitzky-Golay	4	0.57	0.84	0.53	0.82
	1st Derivative	3	0.62	0.80	0.55	0.81
	2nd Derivative	3	0.60	0.81	0.56	0.80
	MSC	7	0.71	0.72	0.49	0.86

3.3 Models of quality indices

Support vector machines (SVM) are learning algorithms that present good generalization performance and can model complex non linear boundaries through use of adapted kernel functions[19, 20]. Back propagation neural network (BPNN) is one of the most widely used mathematical algorithms for overcoming non-linearity[21]. The models were developed by SVM, BPNN and partial least squares (PLS), respectively. PLS can easily treat very large data matrices, extract the relevant part of the information and produce reliable but very complex models[22]. The code of SVM was downloaded from the website (www.isis.ecs.soton.ac.uk/resources/ svminfo). The NIR spectra were treated by principal component analysis (PCA). The scores of PCA were used as the input vector for SVM and BPNN. The SVM parameters of kernel function and penalty factor were Sigmoid and C = 2×10^3, respectively. The three networks were adopted and were trained by Levenberg-Marquardt training algorithm[23]. The number of hidden nodes was 9 after testing. The performance of models were compared, which were built by SVM, BP and PLS (Table 3), respectively. The results indicated better model performance when using SVM.

Table 3 Comparison of regression results among SVM, BP and PLS

Indices	Modeling methods	Calibration set		Prediction set	
		R	*RMSEC*	*R*	*RMSEP*
SSC	SVM	0.95	0.52	0.93	0.65
	BPNN	0.95	0.52	0.93	0.64
	PLS	0.94	0.53	0.92	0.65
TA	SVM	0.67	0.09	0.66	0.09
	BPNN	0.67	0.09	0.65	0.09
	PLS	0.65	0.10	0.64	0.09
Vitamin C	SVM	0.81	3.20	0.81	2.70
	BPNN	0.80	3.20	0.80	2.70
	PLS	0.80	3.30	0.80	2.80
Surface color	SVM	0.57	0.82	0.57	0.81
	BPNN	0.57	0.82	0.54	0.81
	PLS	0.57	0.84	0.53	0.82

3.3.1 Soluble solids content

The better result of model was obtained by SVM for SSC. The R of calibration model was 0.95 with the RMSEC of 0.52°Brix. When the model was used to predict the 43 unknown samples, the R of prediction model was 0.93 with the RMSEP of 0.65°Brix. The model of SSC is shown in Figure 3.

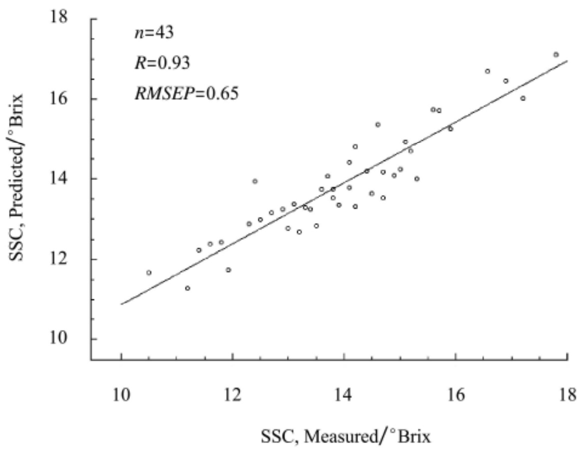

Figure 3 Predicted model of SSC

The RMSEP obtained in this research is lightly superior to those obtained by Camps et al. (2009) with RMSEP=0.67−1.10°Brix in apricot by a portable visible-near infrared spectroscopy[15] and Liu et al. (2008) with RMSEP=0.66°Brix in pear by a research instrument[24]. But better results have been found in mango with SEP=0.40°Brix by "Fruit Tester 20" (FANTEC, Kosai-city, Japan) and "Model 6500" (Foss NIRSystems, Silver Sping, USA)[13], in apple with SEP = 0.46°Brix by FT-NIR spectrometer (Thermo Nicolet Corporation, USA)[25] and in mandarin fruit with RMSEP = 0.33°Brix by a research instrument[11].

3.3.2 TA

The R of calibration model was 0.67 with the RMSEC of 0.09%. When the model was used to predict the 42 unknown samples, the R of prediction model was 0.66 with the RMSEP of 0.09%. The model of SSC is shown in Figure 4. A better result was obtained with SEP = 0.04% by FT-NIR spectrometer (Thermo Nicolet Corporation, USA)[25].

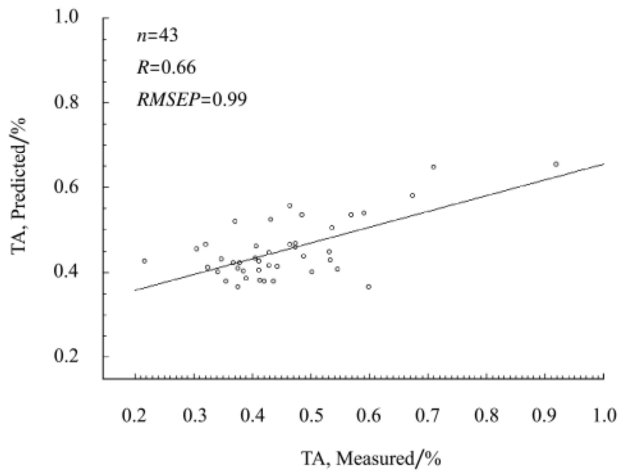

Figure 4 Predicted model of TA

3.3.3 Vitamin C

The R of calibration model was 0.81 with the RMSEC of 3.2 mg/(100 g). When the model was used to predict the 41 unknown samples, the R of prediction model was 0.81 with the RMSEP of 2.7 mg/(100 g). The model of SSC is shown in Figure 5. The result obtained in this research is lightly superior to the result with RMSEP = 3.9 mg/(100 g) in orange[26]. But it is not better than Liu et al. (2008) with RMSEP = 2.1 mg/(100 g) in mandarin fruit by a research instrument[27].

3.3.4 Color

The R of calibration model was 0.57 with the RMSEC of 0.82. When the model was used to predict the 37 unknown samples, the R of prediction model was 0.57 with the RMSEP of 0.81. The model of SSC is shown in Figure 6.

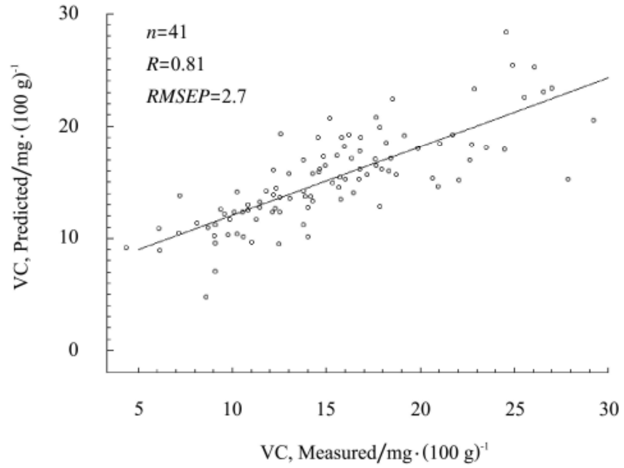

Figure 5 Predicted model of vitamin C

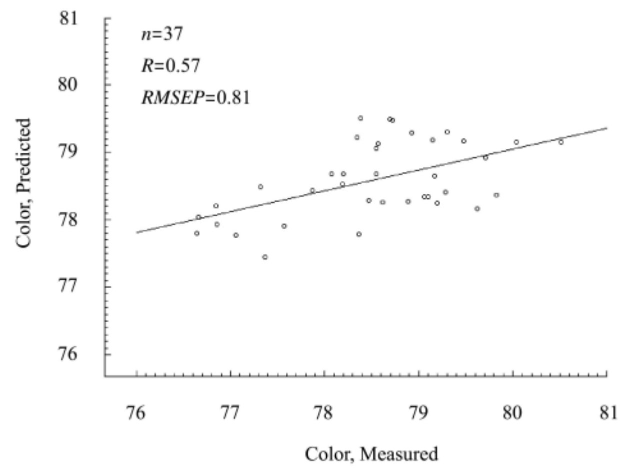

Figure 6 Predicted model of $\triangle E$

4 Conclusions

A portable near infrared spectroscopy system was developed to determine the quality of Nanfeng mandarin fruit nondestructively. Better models were obtained by SVM for quality indices of Nanfeng mandarin fruit, including SSC, TA, vitamin C and color. It is possible to assess the Nanfeng mandarin quality nondestructively by the portable near infrared spectroscopy system.

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